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=> display history full 11-FILE 'REGISTRY' ENTERED AT 16:59:27 ON 08 MAR 2006 E CELLULOSE/CN L11 SEA CELLULOSE/CN E STARCH/CN L2 1 SEA STARCH/CN FILE 'HCA' ENTERED AT 17:04:05 ON 08 MAR 2006 828873 SEA L1 OR L2 OR CELLULOS? OR CELLULOLY? OR STARCH? OR L3 ?SACCHARID? OR ?CARBOHYDRAT? OUE HALIDE# OR BROMIDE# OR CHLORIDE# OR IODIDE# OR L4HYPOHALITE# OR HYPOCHLORITE# OR HYPOBROMITE# OR HYPOIODIT E# FILE 'REGISTRY' ENTERED AT 17:04:24 ON 08 MAR 2006 E PEROXIDASE/CN L5 1 SEA PEROXIDASE/CN E LACTOPEROXIDASE/CN L6 1 SEA LACTOPEROXIDASE/CN E MYELOPEROXIDASE/CN 1 SEA MYELOPEROXIDASE/CN L7 E HALOPEROXIDASE/CN 1 SEA HALOPEROXIDASE/CN L8 L9 2 SEA (L5 OR L6 OR L7 OR L8) FILE 'HCA' ENTERED AT 17:08:15 ON 08 MAR 2006 L10 91168 SEA L9 OR ?PEROXIDAS? L116285 SEA (NITROXYL# OR NITROSONIUM# OR TEMPO OR PROXYL OR DOXYL OR N(W)OXIDE#) AND RADICAL? FILE 'LREGISTRY' ENTERED AT 17:09:18 ON 08 MAR 2006 E NITROSYL L12 1 SEA NITROSYLBENZENE/BI FILE 'HCA' ENTERED AT 17:10:40 ON 08 MAR 2006

4565 SEA (NITROSYL? OR NITROSO?) AND RADICAL?

FILE 'LREGISTRY' ENTERED AT 17:10:51 ON 08 MAR 2006

STR

L13

L14

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E NITROXYL
L15
             9 SEA NITROXYL/BI
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L16
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L17
L18
               STR L14
            50 SEA SSS SAM L18
L19
L20 33723 SEA SSS FUL L18
               SAV TEM L20 HUG069/A
L21
        53800 SEA RADICAL?
L22
          152 SEA L20 AND L21
            34 SEA C12H24N3O2
L23
L24
             1 SEA L22 AND L23
     FILE 'HCA' ENTERED AT 17:28:55 ON 08 MAR 2006
L25
          6754 SEA L22
          8669 SEA L20 AND RADICAL?
L26
          481 SEA L3 AND L4 AND L10
L27
L28
            1 SEA L27 AND L11
             1 SEA L27 AND L13
L29
             2 SEA L27 AND L16
L30
L31
             5 SEA L27 AND L25
            2 SEA L27 AND L26
L32
L33
        28913 SEA L20
            10 SEA L27 AND L33
L34
L35
            8 SEA (L28 OR L29 OR L30 OR L31 OR L32)
            19 SEA L3 AND L10 AND (L11 OR L13 OR L16 OR L25 OR L26)
L36
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L37
               ?BROMID? OR ?IODID? OR ?HYPOHALID? OR ?HYPOFLUORID? OR
               ?HYPOCHLORID? OR ?HYPOBROMID? OR ?HYPOIODID?
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             4 SEA L36 AND L37
L38
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L39
           432 SEA HYPOCHLORITE# OR HYPOBROMITE# OR HYPOIODITE#
L40
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L41 281662 SEA L39 OR L40
L42
             3 SEA L36 AND L41
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FILE 'REGISTRY' ENTERED AT 17:53:53 ON 08 MAR 2006

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8635 SEA M/ELS (L) X/ELS (L) 2/ELC.SUB
L43
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L44
              2 SEA L36 AND L44
L45
L46
              8 SEA L35 OR L38 OR L42 OR L45
              6 SEA L34 AND L46
L47
              8 SEA L46 OR L47
L48
              4 SEA L34 NOT L48
L49
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=> d 120 que stat
L18
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1 2 3
NODE ATTRIBUTES:
HCOUNT IS EO
                AΤ
NSPEC
       IS RC
                  AT
       IS RC
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NSPEC
CONNECT IS E1 RC AT
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 4
STEREO ATTRIBUTES: NONE
L20
         33723 SEA FILE=REGISTRY SSS FUL L18
100.0% PROCESSED 218591 ITERATIONS
                                                            33723 ANSWERS
SEARCH TIME: 00.00.01
=> file hca
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=> d 148 1-8 cbib abs hitstr hitind

L48 ANSWER 1 OF 8 HCA COPYRIGHT 2006 ACS on STN

141:381254 Crystalline polysaccharide derivatives, their production and their applications. Vignon, Michel; Montanari, Suzelei; Habibi, Youssef (Centre National de la Recherche Scientifique CNRS, Fr.). Fr. Demande FR 2854161 A1 20041029, 68 pp. (French). CODEN: FRXXBL. APPLICATION: FR 2003-5195 20030428.

The invention relates to cryst. polysaccharide derivs. in which at least part of the CH2OH groups are oxidized to CO2H groups, whereby the latter are able to be partly or entirely in the form of salts or functionalized. These derivs. are characterized in that they are present in the form of aggregates comprising microcrystals and/or individualized microfibrils, with the lateral sizes of the microcrystals and microfibrils being on the order of 1-30 nm and their length up to .apprx.100 .mu.m, whereby the the microcrystals and microfibrils form aggregates in water. The products may be used as viscosifiers, stabilizers, superabsorbents, or chelators. In an example, cotton linters were oxidized with NaOCl in the presence of TEMPO and NaBr. Other examples deal with starch and chitin.

IT 2226-96-2, 4-Hydroxy-TEMPO 2564-83-2, TEMPO 6599-87-7, 4-Acetoxy-TEMPO 7647-15-6, Sodium bromide, uses 9003-99-0, Peroxidase 14691-88-4, 4-Amino-TEMPO 14691-89-5, 4-Acetamido-TEMPO 15178-63-9, 4-Maleimido-TEMPO 22690-04-6, 4-(Phosphonooxy)-TEMPO 31645-22-4, 4-(Benzyloxy)-TEMPO (in prodn. of microcryst. and microfibrillar oxidized polysaccharide derivs.)

RN 2226-96-2 HCA

CN 1-Piperidinyloxy, 4-hydroxy-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

RN 2564-83-2 HCA

CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

RN 6599-87-7 HCA

CN 1-Piperidinyloxy, 4-(acetyloxy)-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

RN 7647-15-6 HCA

CN Sodium bromide (NaBr) (9CI) (CA INDEX NAME)

Br-Na

RN 9003-99-0 HCA

CN Peroxidase (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 14691-88-4 HCA

CN 1-Piperidinyloxy, 4-amino-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

RN 14691-89-5 HCA

CN 1-Piperidinyloxy, 4-(acetylamino)-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

RN 15178-63-9 HCA

CN 1-Piperidinyloxy, 4-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

RN 22690-04-6 HCA

CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl-4-(phosphonooxy)- (9CI) (CA INDEX NAME)

RN 31645-22-4 HCA

CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)

IT 7681-52-9, Sodium hypochlorite

(in prodn. of microcryst. and microfibrillar oxidized polysaccharide derivs.)

RN 7681-52-9 HCA

CN Hypochlorous acid, sodium salt (8CI, 9CI) (CA INDEX NAME)

C1-OH

Na

9004-34-6DP, Cellulose, oxidized IT 9005-25-8DP, Starch, oxidized (prodn. of microcryst. and microfibrillar oxidized polysaccharide derivs.) 9004-34-6 HCA RN Cellulose (8CI, 9CI) (CA INDEX NAME) CN*** STRUCTURE DIAGRAM IS NOT AVAILABLE *** 9005-25-8 HCA RN Starch (8CI, 9CI) (CA INDEX NAME) CN *** STRUCTURE DIAGRAM IS NOT AVAILABLE *** ICM C08B015-00 IC 43-3 (Cellulose, Lignin, Paper, and Other Wood Products) CC Section cross-reference(s): 44 polysaccharide oxidn microcryst microfiber product; ST cellulose starch chitin oxidn microcryst microfiber product Rayon, preparation IT (oxidized; in prodn. of microcryst. and microfibrillar oxidized polysaccharide derivs.) IT Linters (prodn. of cryst. oxidized polysaccharide derivs. from) TT Microcrystallites Microfibers (prodn. of microcryst. and microfibrillar oxidized

```
polysaccharide derivs.)
ΙT
     Beta vulgaris saccharifera
        (pulp; in prodn. of microcryst. and microfibrillar oxidized
        polysaccharide derivs.)
TT
     2226-96-2, 4-Hydroxy-TEMPO 2564-83-2, TEMPO
     6599-87-7, 4-Acetoxy-TEMPO 7647-15-6, Sodium
                     9001-62-1, Lipase 9002-10-2, Polyphenol
    bromide, uses
     oxidase 9003-99-0, Peroxidase 14691-88-4
     , 4-Amino-TEMPO 14691-89-5, 4-Acetamido-TEMPO
     15178-63-9, 4-Maleimido-TEMPO 22690-04-6,
     4-(Phosphonooxy)-TEMPO 31645-22-4, 4-(Benzyloxy)-TEMPO
     80498-15-3, Laccase
        (in prodn. of microcryst. and microfibrillar oxidized
        polysaccharide derivs.)
     100-46-9DP, Benzylamine, reaction products with oxidized
IΤ
                 109-85-3DP, 2-Methoxyethylamine, reaction
                                        110-60-1DP,
     products with oxidized cellulose
     1,4-Diaminobutane, reaction products with oxidized cellulose
     9037-22-3DP, Waxilys, oxidized 25189-55-3DP, Poly(N-
     isopropylacrylamide), reaction products with oxidized
     cellulose 111144-84-4DP, reaction products with oxidized
     cellulose
                 783344-73-0DP, reaction products with oxidized
     cellulose
        (in prodn. of microcryst. and microfibrillar oxidized
        polysaccharide derivs.)
     67-56-1, Methanol, uses
                             1892-57-5, EDAC
IT
        (in prodn. of microcryst. and microfibrillar oxidized
        polysaccharide derivs.)
     7681-52-9, Sodium hypochlorite 10028-15-6,
IT
     Ozone, reactions
        (in prodn. of microcryst. and microfibrillar oxidized
        polysaccharide derivs.)
                                     9000-07-1DP, Carrageenan, oxidized
     1398-61-4DP, Chitin, oxidized
IT
     9004-34-6DP, Cellulose, oxidized
     9005-25-8DP, Starch, oxidized
                                     9005-80-5DP,
     Inulin, oxidized 9005-82-7DP, Amylose, oxidized Agarose, oxidized 9012-72-0DP, Glucan, oxidized
                                                          9012-36-6DP,
                                                          9014-63-5DP,
     Xylan, oxidized 9036-88-8DP, Mannan, oxidized 31799-84-5DP,
     Nigeran, oxidized
        (prodn. of microcryst. and microfibrillar oxidized
        polysaccharide derivs.)
    ANSWER 2 OF 8 HCA COPYRIGHT 2006 ACS on STN
139:391295 Do stable nitroxide radicals catalyze or
     inhibit the degradation of hyaluronic acid?. Lurie, Ziva; Offer,
     Tal; Russo, Angelo; Samuni, Amram; Nitzan, Dorrit (Department of
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Molecular Biology, Hebrew University-Hadassah Medical School,

Jerusalem, Israel). Free Radical Biology & Medicine, 35(2), 169-178

(English) 2003. CODEN: FRBMEH. ISSN: 0891-5849. Publisher: Elsevier Science Inc..

Reactive oxygen-derived species and particularly OH radicals can degrade hyaluronic acid (HA), resulting in a loss of viscosity and a subsequent decrease in its effectiveness as a joint-lubricating agent. The prodn. of OH in the vicinity of HA can be catalyzed by bound redox-active metals, which participate in the Haber-Weiss reaction. Damage to HA can also occur as a result of hypochlorite formed by myeloperoxidase (MPO). protective reagents commonly used to inhibit oxidative stress-induced degrdn. of HA include antioxidative enzymes, such as SOD and catalase, chelators that coordinate metal ions rendering them redox-inactive, and scavengers of radicals, such as OH, as well as nonradical reactive species. In recent years, stable cyclic nitroxides have also been widely used as effective antioxidants. In many cases, nitroxide antioxidants operate catalytically and mediate their protective effect through an exchange between their oxidized and reduced forms. It was anticipated, therefore, that nitroxides would protect HA from oxidative degrdn. as well. On the other hand, nitroxides serve as catalysts in many oxidn. reactions of alcs., sugars and polysaccharides, including hyalouronan. Such opposite effects of nitroxides on oxidative degrdn. are particularly intriguing and the aim of the present study was to examine their effect on HA when subjected to diverse forms of oxidative stress. The results indicate that nitroxides protect HA from OH radicals generated enzymically or radiolytically. The protective effect is attributable neither to the scavenging of OH nor to the oxidn. of reduced metal, but to the reaction of nitroxides with secondary carbohydrate radicals-most likely peroxyl radicals.

2226-96-2, 4-Hydroxy-2,2,6,6-tetramethyl piperidine-1-oxyl 2564-83-2, 2,2,6,6-Tetra-methyl piperidine-1-oxyl 14691-88-4, 4-Amino-2,2,6,6-tetra-methyl piperidine-1-oxyl (stable nitroxide radicals effect on degrdn. of hyaluronic acid)

RN 2226-96-2 HCA

CN 1-Piperidinyloxy, 4-hydroxy-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

AB

RN 2564-83-2 HCA

CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

RN 14691-88-4 HCA

CN 1-Piperidinyloxy, 4-amino-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

CC 1-12 (Pharmacology)

Section cross-reference(s): 8, 14

ST **nitroxide** antioxidant superoxide SOD mimetic ionizing radiation hyaluronate viscosity; antiinflammatory rheumatoid arthritis **nitroxide** hyaluronate oxidative stress free radical

IT Anti-inflammatory agents

Antioxidants

Antirheumatic agents

Gamma ray

Rheumatoid arthritis

Viscosity

(stable nitroxide radicals effect on degrdn.

of hyaluronic acid)

IT Radicals, biological studies

(stable nitroxide radicals effect on degrdn.

of hyaluronic acid)

IT Nitroxides

(stable nitroxide radicals effect on degrdn.

of hyaluronic acid)

IT 9054-89-1

(copper-zinc-contg.; stable nitroxide radicals

effect on degrdn. of hyaluronic acid) IT 3352-57-6, Hydroxyl, biological studies 7722-84-1, Hydrogen 14337-01-0, peroxide, biological studies 11062-77-4, Superoxide biological studies (stable nitroxide radicals effect on degrdn. of hyaluronic acid) 9004-61-9, Hyaluronic acid ΙT (stable nitroxide radicals effect on degrdn. of hyaluronic acid) 69-65-8, Mannitol 70-51-9, Desferrioxamine 68-94-0, Hypoxanthine IT **2226-96-2**, 4-Hydroxy-2,2,6,6-tetramethyl piperidine-1-oxyl **2564-83-2**, 2,2,6,6-Tetra-methyl piperidine-1-oxyl 9001-05-2, Catalase 9002-17-9 **14691-88-4**, 4-Amino-2,2,6,6-tetra-methyl piperidine-1-oxyl (stable nitroxide radicals effect on degrdn. of hyaluronic acid) ANSWER 3 OF 8 HCA COPYRIGHT 2006 ACS on STN L48 138:155270 Process for the selective modification of carbohydrates by peroxidase catalyzed oxidation. Cui, Xiaoyuan; Cimecioglu, A. Levent; Shi, Yong-Cheng (USA). U.S. Pat. Appl. Publ. US 2003029588 A1 20030213, 7 pp. (English). CODEN: USXXCO. APPLICATION: US 2001-851069 20010508. The present invention relates to an environmentally friendly process AB The process for the selective oxidn. of carbohydrates. comprises the addn. of a hydroperoxide, including hydrogen peroxide, to a carbohydrate having primary alc. groups, particularly including polysaccharides, wherein said carbohydrate is contact with a nitroxyl radical mediator and the process is catalyzed by a peroxidase enzyme in the presence of halide ions. Thus, 50 g Amioca starch was added to 200 mL water in which 0.5 g 4-acetamido-TEMPO, 0.5 g NaBr and 20 mg lactoperoxidase (4.times.600 units, L-8257) were dissolved. The mixt. was incubated at room temp. at an initial pH of 5.3, and 0.5% H2O2 was slowly added (30 .mu.L/min). The pH of the reaction was initially increased from 5.3 to 6.5 and maintained at 6.5 by the slow addn. of NaOH (0.1 N). After 20 h, 0.56 mL of 0.1 N NaOH was The starch slurry was then filtered and consumed. starch cake was reslurried in water 4 times (200 mL each) until no detectable H2O2 remained in the filtrate, and then The oxidized Amioca starch showed an aldehyde air-dried. content 0.34%. 7647-15-6, Sodium bromide, reactions IT (halide ion source; process for selective modification of carbohydrates by peroxidase catalyzed oxidn. in the presence of nitroxyl radical) 7647-15-6 HCA RN

CN Sodium bromide (NaBr) (9CI) (CA INDEX NAME)

Br-Na

IT 9003-99-0, Lactoperoxidase 14691-89-5,

4-Acetamido-TEMPO

(process for selective modification of **carbohydrates** by **peroxidase** catalyzed oxidn. in the presence of **nitroxyl radical**)

RN 9003-99-0 HCA

CN Peroxidase (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 14691-89-5 HCA

CN 1-Piperidinyloxy, 4-(acetylamino)-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

IC ICM D21C009-00

ICS D21C003-20; D06M023-00; D06M013-322

INCL 162072000; 162009000; 162157600; 162109000; 008120000; 008181000; 008116100

CC 44-6 (Industrial Carbohydrates)

Section cross-reference(s): 7, 33, 43

ST lactoperoxidase nitroxyl radical oxidn

polysaccharide carbohydrate aldehyde manuf

IT Enzymes, uses

(peroxidases; process for selective modification of carbohydrates by peroxidase catalyzed oxidn. in

the presence of nitroxyl radical)

IT Cellulose pulp

(process for selective modification of **carbohydrates** by **peroxidase** catalyzed oxidn. in the presence of **nitroxyl radical**)

IT 7647-15-6, Sodium bromide, reactions

(halide ion source; process for selective modification

of carbohydrates by peroxidase catalyzed

oxidn. in the presence of nitroxyl radical)

IT 7722-84-1, Hydrogen peroxide, reactions (oxidant; process for selective modification of

carbohydrates by peroxidase catalyzed oxidn. in
the presence of nitroxyl radical)

IT 3149-68-6DP, Methyl glucoside, oxidized product 9037-22-3DP, Amioca, oxidized products

(process for selective modification of carbohydrates by peroxidase catalyzed oxidn. in the presence of nitroxyl radical)

9003-99-0, Lactoperoxidase 9031-28-1, Thyroid peroxidase 14691-89-5, 4-Acetamido-TEMPO

(process for selective modification of **carbohydrates** by **peroxidase** catalyzed oxidn. in the presence of **nitroxyl radical**)

- IT 3149-68-6, Methyl glucoside 9037-22-3, Amioca (process for selective modification of carbohydrates by peroxidase catalyzed oxidn. in the presence of nitroxyl radical)
- ANSWER 4 OF 8 HCA COPYRIGHT 2006 ACS on STN L48 138:124179 Extraction of polysaccharides from vegetable and microbial material using oxidizing agents. Van Der Wilden, Wim; Haaksman, Ingrid Karin; Ekhart, Peter Frank; Jetten, Jan Matthijs (Nederlandse Organisatie Voor Toegepast-Natuurwetenschappelijk Onderzoek Tno, Neth.). PCT Int. Appl. WO 2003008458 A1 20030130, 15 DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, pp. BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2002-NL482 20020717. PRIORITY: NL 2001-1018568
- AB Useful polysaccharides, such as .beta.-1,3-glucans, from a biol. raw material can be solubilized and/or isolated by treating the raw material with an oxidizing agent that leads to oxidn. of primary hydroxyl groups in the glucan. The oxidizing agent is preferably a catalytic amt. of a nitroxyl compd. in the presence of a re-oxidizing agent such as hypochlorite or an oxidative enzyme with oxygen or hydrogen peroxide. The polysaccharide retains its useful properties during this treatment and is, moreover, more readily available. If desired, protein material from the raw material can also be utilized.
- IT **2564-83-2**, TEMPO

(extn. of **polysaccharides** from vegetable and microbial material using oxidizing agents)

- RN 2564-83-2 HCA
- CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

9003-99-0, Peroxidase IT (oxidizing agent; extn. of polysaccharides from vegetable and microbial material using oxidizing agents) RN 9003-99-0 HCA Peroxidase (9CI) (CA INDEX NAME) CN *** STRUCTURE DIAGRAM IS NOT AVAILABLE *** C08B037-00; C07H003-06 IC 44-5 (Industrial Carbohydrates) CC ST polysaccharide extn oxidizing agent ΙT Binders Emulsifying agents Oxidation Oxidizing agents Wetting agents (extn. of polysaccharides from vegetable and microbial material using oxidizing agents) IT Yeast (flakes; extn. of polysaccharides from vegetable and microbial material using oxidizing agents) Polysaccharides, preparation IT (oxidized; extn. of polysaccharides from vegetable and microbial material using oxidizing agents) IT Beta vulgaris saccharifera (pulp; extn. of polysaccharides from vegetable and microbial material using oxidizing agents) IT Cereal (grain) (residues; extn. of polysaccharides from vegetable and microbial material using oxidizing agents) 7790-92-3, Hypochlorous acid **2564-83-2**, TEMPO IT(extn. of polysaccharides from vegetable and microbial material using oxidizing agents) 9002-10-2, Polyphenol oxidase 9003-99-0, IT 80498-15-3, Laccase Peroxidase (oxidizing agent; extn. of polysaccharides from vegetable and microbial material using oxidizing agents) ANSWER 5 OF 8 HCA COPYRIGHT 2006 ACS on STN

137:105054 Nitrosation and Nitration of 2-Amino-3-methylimidazo[4,5-f

]quinoline by Reactive Nitrogen Oxygen Species. Lakshmi, Vijaya M.;

Hsu, Fong Fu; Zenser, Terry V. (Division of Geriatric Medicine, VA Medical Center, St. Louis, MO, 63125, USA). Chemical Research in Toxicology, 15(8), 1059-1068 (English) 2002. CODEN: CRTOEC. ISSN: 0893-228X. Publisher: American Chemical Society.

Both cooked red meat intake and chronic inflammation/infection are AB thought to play a role in the etiol. of colon cancer. heterocyclic amine 2-amino-3-methylimidazo[4,5-f]quinoline (IQ) is formed during cooking of red meat and may be involved in initiation of colon cancer. Reactive nitrogen oxygen species (RNOS), components of the inflammatory response, contribute to the deleterious effects attributed to inflammation on normal tissues. This study assessed the possible chem. transformation of IQ by RNOS. RNOS were generated by various conditions to react with C-IQ, and samples were evaluated by HPLC. Myeloperoxidase (MPO) -catalyzed reaction was dependent upon both H2O2 and NO2-. This reaction produced an azo-IQ dimer and IQ dimer along with two nitrated IQ products identified by ESI/MS. 2-Nitro-IQ was not detected. Product formation was inhibited by 2 mM cyanide. in nitrated products obsd. with 100 mM chloride was not altered with 0.5 mM taurine. Nitrated products were also produced by other conditions, ONOO- and NO2- + HOCl, which generate nitrogen dioxide radical. In contrast, conditions which generate N2O3, such as diethylamine NONOate, produced only small amts. of nitrated products with the major product identified by MS and NMR as N-nitroso-IQ. MPO activation of IQ to bind DNA was dependent upon both H2O2 and NO2-. RNOS generated by ONOO- and DEA NONOate also activated IQ DNA binding. The nitrated IQ products were not activated by MPO to bind DNA. In contrast, Nnitroso-IO was activated to bind DNA by MPO .+-. NO2-. HOCl activated N-nitroso-IQ, but not IQ. RAW cells produced Nnitroso-IQ and increased amts. of NO2-/NO3-, when incubated with 0.1 mM IQ and stimulated with lipopolysaccharide and interferon gamma. Results demonstrate chem. transformation and activation of IQ by RNOS and activation of its N-nitroso product by biol. oxidants, events which may contribute to initiation of colon cancer.

9003-99-0, Myeloperoxidase

(nitrosation and nitration of IQ by reactive nitrogen oxygen species)

RN 9003-99-0 HCA

ΙT

- CN Peroxidase (9CI) (CA INDEX NAME)
- *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
- CC 4-6 (Toxicology)

Section cross-reference(s): 17

IT 9003-99-0, Myeloperoxidase 76180-96-6, 2-Amino-3-methylimidazo[4,5-f] quinoline 146724-94-9, Diethylamine NONOate

(nitrosation and nitration of IQ by reactive nitrogen oxygen

species)

NAME)

```
ANSWER 6 OF 8 HCA COPYRIGHT 2006 ACS on STN
L48
133:209532 Oxidized cellulose-containing fibrous materials,
     preparation thereof and products therefrom. Jaschinski, Thomas;
     Gunnars, Susanna; Besemer, Arie Cornelis; Bragd, Petter; Jetten, Jan
     Matthijs; Van den Dool, Ronald; Van Hartingsveldt, Willem (Sca
     Hygiene Products G.m.b.H., Germany; Sca Hygiene Products Zeist
            PCT Int. Appl. WO 2000050462 Al 20000831, 75 pp.
                                                               DESIGNATED
                AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN,
     STATES: W:
     CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID,
     IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
     MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK,
     SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY,
     KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY,
     DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT,
     SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO
     2000-EP1538 20000224.
                           PRIORITY: EP 1999-200537 19990224; DE
     1999-19953590 19991108.
     A cellulose-contq. fibrous material is prepd. by oxidizing
AΒ
     hydroxy groups at the C(6) of glucose units of cellulose
     into aldehyde and/or carboxy groups, and used to prep. paper or
     nonwoven products, esp. tissue products. The paper or nonwoven
     products display excellent strength properties. Thus, bleached
     hardwood sulfite pulp was treated for 60 min under acidic conditions
     with 4-hydroxy-TEMPO (1.00 g/50 g dry fibrous material) using 5% of
     13% NaOCl as a primary oxidizing agent, and used to prep. test
     sheets (basis wt. 80 g/m2) having wt. 2.56 g, breaking strength
     23.94 (dry) and 4.687 N/15 mm (wet), tear length 1980.1 (dry) and
     387.7 m (wet), and rel. wet strength 19.6%, compared with 3.04,
     18.48, 0.151, 1285.7, 10.5, and 0.8, resp., for a nonoxidized pulp.
     9004-34-6DP, Cellulose, oxidized, preparation
IT
        (contg. aldehyde and/or carboxyl groups; oxidized
        cellulose-contq. fibrous materials, prepn. thereof and
        products therefrom)
RN
     9004-34-6 HCA
CN
     Cellulose (8CI, 9CI) (CA INDEX NAME)
***
    STRUCTURE DIAGRAM IS NOT AVAILABLE ***
ΙT
     2226-96-2, 4-Hydroxy-TEMPO 2564-83-2, TEMPO
     9003-99-0, Peroxidase 14691-88-4,
     4-Amino-TEMPO 14691-89-5, 4-Acetamido-TEMPO
        (oxidized cellulose-contq. fibrous materials, prepn.
        thereof and products therefrom)
RN
     2226-96-2
               HCA
     1-Piperidinyloxy, 4-hydroxy-2,2,6,6-tetramethyl- (9CI) (CA INDEX
CN
```

RN 2564-83-2 HCA

CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

RN 9003-99-0 HCA

CN Peroxidase (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 14691-88-4 HCA

CN 1-Piperidinyloxy, 4-amino-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

RN 14691-89-5 HCA

CN 1-Piperidinyloxy, 4-(acetylamino)-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

IT 7681-52-9, Sodium hypochlorite

(oxidized cellulose-contg. fibrous materials, prepn.

thereof and products therefrom)

RN 7681-52-9 HCA

CN Hypochlorous acid, sodium salt (8CI, 9CI) (CA INDEX NAME)

C1-OH

Na

IC ICM C08B015-02

ICS C08B015-04; D21H011-20

CC 43-7 (Cellulose, Lignin, Paper, and Other Wood Products)

ST cellulose oxidn aldehydocellulose carboxycellulose paper strength; sodium hypochlorite TEMPO oxidn

cellulose; piperidinyloxy sodium hypochlorite

oxidn cellulose

IT Household furnishings

(bedding; oxidized **cellulose**-contg. fibrous materials, prepn. thereof and products therefrom)

IT Cellulose pulp

(kraft; oxidized **cellulose**-contg. fibrous materials, prepn. thereof and products therefrom)

IT Oxidizing agents

(metal-contg.; oxidized **cellulose**-contg. fibrous materials, prepn. thereof and products therefrom)

IT Clothing

Nonwoven fabrics

(oxidized **cellulose**-contg. fibrous materials, prepn. thereof and products therefrom)

IT Hypohalites

Peroxy acids

(oxidized **cellulose**-contg. fibrous materials, prepn. thereof and products therefrom)

IT Cellulose pulp

(sulfite; oxidized cellulose-contg. fibrous materials, prepn. thereof and products therefrom) ΙT Paper (tissue, facial; oxidized cellulose-contg. fibrous materials, prepn. thereof and products therefrom) IT Paper (tissue; oxidized cellulose-contg. fibrous materials, prepn. thereof and products therefrom) IT Paper (towels; oxidized cellulose-contg. fibrous materials, prepn. thereof and products therefrom) IT Medical goods (wipes; oxidized cellulose-contg. fibrous materials, prepn. thereof and products therefrom) IT Household furnishings (wiping cloths; oxidized cellulose-contg. fibrous materials, prepn. thereof and products therefrom) 9004-34-6DP, Cellulose, oxidized, preparation IT (contg. aldehyde and/or carboxyl groups; oxidized cellulose-contg. fibrous materials, prepn. thereof and products therefrom) IT 39301-50-3P, 6-Aldehydocellulose (oxidized cellulose-contg. fibrous materials, prepn. thereof and products therefrom) 2226-96-2, 4-Hydroxy-TEMPO 2564-83-2, TEMPO IT 9003-99-0, Peroxidase 14691-88-4, 4-Amino-TEMPO 14691-89-5, 4-Acetamido-TEMPO (oxidized cellulose-contg. fibrous materials, prepn. thereof and products therefrom) 7681-52-9, Sodium hypochlorite 10028-15-6, IT Ozone, reactions (oxidized cellulose-contg. fibrous materials, prepn. thereof and products therefrom) ANSWER 7 OF 8 HCA COPYRIGHT 2006 ACS on STN 130:326478 Method for modification of cellulose. Viikari, Liisa; Kruus, Kristiina; Buchert, Johanna (Valtion Teknillinen Tutkimuskeskus, Finland). PCT Int. Appl. WO 9923117 A1 19990514, 16 DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-FI861 19981104. PRIORITY: FI 1997-4139 19971104.

The method comprises bringing a cellulose-contg. material

AB

(pine kraft pulp) into contact with a reactant (e.g., 2,2,6,6-tetramethylpiperidine-1-oxyl) producing an oxoammonium ion in the presence of an oxidizing agent (e.g., laccase). The invention provides selective oxidn., which gives rise to the formation of carboxylic and carbonyl groups at desired ratios in the cellulose. By using laccase it is possible to avoid the environmentally harmful halide-contg. materials commonly used as oxidants.

IT 9003-99-0, Peroxidase

(method for modification of cellulose)

RN 9003-99-0 HCA

CN Peroxidase (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT **2564-83-2**, TEMPO

(method for modification of cellulose)

RN 2564-83-2 HCA

CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

IC ICM C08B015-04

ICS C12S003-00; D21C009-10

CC 43-3 (Cellulose, Lignin, Paper, and Other Wood Products)

IT Cellulose pulp

(kraft; method for modification of cellulose)

IT Oxidizing agents

(method for modification of cellulose)

IT Cellulose pulp

(oxidized; method for modification of cellulose)

IT Enzymes, uses

(oxidizing, oxidizing agents; method for modification of cellulose)

IT **9003-99-0**, **Peroxidase** 80498-15-3, Laccase

(method for modification of cellulose)

IT **2564-83-2**, TEMPO 7722-84-1, Hydrogen peroxide, uses (method for modification of **cellulose**)

L48 ANSWER 8 OF 8 HCA COPYRIGHT 2006 ACS on STN

119:173983 Oxidation of desferrioxamine to **nitroxide** free **radical** by activated human neutrophils. Soriani, Marco; Mazzuca, Silvia; Quaresima, Valentina; Minetti, Maurizio (Lab. Biol. Cell., Ist. Super. Sanita, Rome, 00161, Italy). Free Radical

Biology & Medicine, 14(6), 589-99 (English) 1993. CODEN: FRBMEH. ISSN: 0891-5849.

Human neutrophils activated by PMA were found to induce the formation of a nitroxide radical from DFO. presence of SOD was necessary to permit the formation of the DFO radical. The inactive phorbol ester did not induce DFO radical, and DL-sphinganine suppressed the radical produced by the active phorbol ester. Other cell stimuli (Zymocel and the chemotactic peptide) also induced the formation of the DFO radical, although radical concn. was very much lower than with PMA. Participation of .bul.NO, .bul.OH or 102 was ruled out by the inability of NG-methyl-L-arginine, NG-nitro-L-arginine, DMSO, mannitol, histidine, and methionine to inhibit the formation of DFO radical produced by PMA-activated cells. Furthermore, PMA-activated cells did not produce detectable levels of NO2-, a stable oxidn. product of .bul.NO, and D2O, which enhances the lifetime of singlet oxygen, did not modify the intensity or the lifetime of DFO radical. The involvement of cell MPO was suggested by the inhibition of the DFO radical obsd. after treatment with catalase or with antihuman MPO antibodies. Also, HOCl was found to induce the DFO radical in cell-free reactions, but this data indicate that the reaction leading to DFO radical formation by neutrophils involves the redn. of MPO compd. II back to the active enzyme (ferric-MPO). Anti-inflammatory drugs strongly increased the DFO radical produced by activated neutrophils. On the contrary, none of these drugs was able to increase the DFO radical produced by HOCl. Histidine and methionine that inhibited the DFO radical intensity in cell-free reactions, were shown to act directly on HOCl. Expts. with MPO-H2O2 in SOD- and Cl--free conditions showed the formation of DFO radical and confirmed the hypothesis of the involvement of compd. II. The conversion of compd. II to ferric MPO by DFO optimized the enzymic activity of neutrophils, and in the presence of monochlorodimedon (compd. II promoting agent) the authors measured an increased HOCl prodn. When DFO was modified by conjugation with hydroxyethyl starch, it lost the ability to produce the radical either by neutrophils or by MPO-H2O2 and did not increase HOCl prodn. The inability of these DFO derivs. to produce potentially toxic species might explain their reported lower toxicity in vivo.

9003-99-0P, Myeloperoxidase

(role in formation of nitroxide free radical,
 in desferrioxamine oxidn., by human neutrophils)
RN 9003-99-0 HCA
CN Peroxidase (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CC 1-10 (Pharmacology)

ΙT

AB

- ST desferrioxamine oxidn **nitroxide** free **radical** neutrophil
- IT Antioxidants

(desferrioxamine as, nitroxide free radical formation by oxidn. of, in neutrophils)

IT Neutrophil

(desferrioxamine oxidn. by, **nitroxide** free **radical** formation in, antioxidant activity in relation to)

IT Hypochlorites

(desferrioxamine oxidn. to **nitroxide radical** by, in human neutrophils, toxicity in relation to)

IT Chelating agents

(desferrioxamine, nitroxide radical formation by oxidn. of, in human neutrophils)

IT Reactive oxygen species

(role in formation of **nitroxide** free **radical**, in desferrioxamine oxidn., by human neutrophils)

IT Inflammation inhibitors

(stimulation of **nitroxide radical** formation in desferrioxamine oxidn. by, in human neutrophils)

IT 70-51-9, Desferrioxamine

(oxidn. of, nitroxide radical formation in, by human neutrophils, antioxidant activity in relation to)

IT 9003-99-0P, Myeloperoxidase

(role in formation of **nitroxide** free **radical**, in desferrioxamine oxidn., by human neutrophils)

- => d 149 1-4 cbib abs hitstr hitind
- L49 ANSWER 1 OF 4 HCA COPYRIGHT 2006 ACS on STN
- 142:444358 Fluorinated resorufin compounds and their application.
 Batchelor, Robert; Ge, Yue; Gee, Kyle; Johnson, Iain; Leung,
 Wai-Yee; Liu, Jixiang; Patch, Brian; Smalley, Peter; Steinberg,
 Thomas (USA). U.S. Pat. Appl. Publ. US 2005096315 A1 20050505, 62
 pp. (English). CODEN: USXXCO. APPLICATION: US 2004-980139
 20041101. PRIORITY: US 2003-2003/PV516244 20031031.
- AB The invention provides novel fluorinated resorufin compds. that are of use in a variety of assay formats. Also provided are methods of using the compds. and kits that include a compd. of the invention and instructions detailing the use of the compd. in one or more assay formats. 2,8-Difluoro-10-acetyl-3,7-dihydroxyphenoxazine (I) was prepd. from 4-fluororesorcinol and isoamyl nitrate in four steps. I was used in enzyme assays for cyclooxygenase 2, Hb, and

glycerol, and in an ELISA for C-reactive protein. IT 9004-34-6, Cellulose, biological studies 9004-34-6D, Cellulose, diazo derivs. 9005-25-8, Starch, biological studies (as solid support linked to fluorinated resorufin compds.; fluorinated resorufin compds. and their use in assays) 9004-34-6 HCA RN Cellulose (8CI, 9CI) (CA INDEX NAME) CN *** STRUCTURE DIAGRAM IS NOT AVAILABLE *** 9004-34-6 HCA RN Cellulose (8CI, 9CI) (CA INDEX NAME) CN*** STRUCTURE DIAGRAM IS NOT AVAILABLE *** RN 9005-25-8 HCA Starch (8CI, 9CI) (CA INDEX NAME) CN *** STRUCTURE DIAGRAM IS NOT AVAILABLE *** IT 851128-88-6P (fluorinated resorufin compds. and their use in assays) 851128-88-6 RN HCA 10H-Phenoxazin-10-yloxy, 2-dodecyl-8-fluoro-3,7-dihydroxy- (9CI) CN (CA INDEX NAME) $(CH_2)_{11}-Me$ HO IT 9003-99-0, Peroxidase (fluorogenic compd. reaction with peroxide in presence of; fluorinated resorufin compds. and their use in assays) 9003-99-0 RN Peroxidase (9CI) (CA INDEX NAME) CN *** STRUCTURE DIAGRAM IS NOT AVAILABLE *** 9003-99-0D, Peroxidase, conjugates with carrier ΙT (fluorogenic compd. reaction with peroxide in presence of; fluorinated resorufin compds. and their use in assays) 9003-99-0 HCA RN Peroxidase (9CI) (CA INDEX NAME) *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 851128-96-6 HCA

851128-96-6P

IT

CN 10H-Phenoxazin-10-yloxy, 2,8-difluoro-3,7-dihydroxy- (9CI) (CA INDEX NAME)

compds. and their use in assays)

(use in detg. cytotoxicity of test compds.; fluorinated resorufin

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IC
     ICM A61K031-5415
          A61K031-538; A61K031-498
     ICS
INCL 514224800; 514229800; 514250000; 544046000; 544102000; 544347000
     9-5 (Biochemical Methods)
CC
     Section cross-reference(s): 7, 15, 28, 41
     Lipopolysaccharides
ΙT
        (Escherichia coli, COX-2 activity induced by, detection of;
        fluorinated resorufin compds. and their use in assays)
     Antibodies and Immunoglobulins
IT
        (IgA, antibody to, conjugates with peroxidase;
        fluorinated resorufin compds. and their use in assays)
IT
     Antibodies and Immunoglobulins
        (IgE, antibody to, conjugates with peroxidase;
        fluorinated resorufin compds. and their use in assays)
     Antibodies and Immunoglobulins
IT
        (IgG, antibody to, conjugates with peroxidase;
        fluorinated resorufin compds. and their use in assays)
     Agglutinins and Lectins
IT
     Amino acids, biological studies
     Antibodies and Immunoglobulins
     Avidins
     Growth factors, animal
     Haptens
     Hormones, animal, biological studies
     Lipids, biological studies
       Lipopolysaccharides
     Nucleic acids
     Nucleosides, biological studies
     Nucleotides, biological studies
     Oligonucleotides
     Peptides, biological studies
     Polymers, biological studies
       Polysaccharides, biological studies
     Proteins
        (as carrier mol. linked to fluorinated resorufin compds.;
        fluorinated resorufin compds. and their use in assays)
     Antibodies and Immunoglobulins
IT
        (conjugates, with horseradish peroxidase; fluorinated
        resorufin compds. and their use in assays)
     Alkyl halides
IT
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Aryl halides

(fluorinated resorufin compds. contg. reactive; fluorinated resorufin compds. and their use in assays) IT Functional groups (silyl, halides, fluorinated resorufin compds. contg. reactive; fluorinated resorufin compds. and their use in assays) Functional groups IT (sulfonyl group, halides, fluorinated resorufin compds. contq. reactive; fluorinated resorufin compds. and their use in IT 9002-18-0, Agar 9002-86-2, Polyvinyl chloride 9002-88-4, Polyethylene 9003-01-4 9003-05-8, Poly(acrylamide) 9003-53-6, Polystyrene **9004-34-6** 9003-07-0, Polypropylene , Cellulose, biological studies 9004-34-6D, 9004-70-0, Nitrocellulose Cellulose, diazo derivs. 9005-25-8, Starch, biological studies 9005-49-6, 9005-79-2, Glycogen, biological Heparin, biological studies 9012-36-6, Sepharose 9036-88-8, studies 9005-80-5, Inulin 25702-74-3, FICOLL 9037-22-3, Amylopectin Mannan (as solid support linked to fluorinated resorufin compds.; fluorinated resorufin compds. and their use in assays) 506-32-1, Arachidonic acid 7647-14-5, ΙT 56-65-5, 5'-ATP, analysis Sodium chloride, analysis 16009-13-5, Hemin (fluorinated resorufin compds. and their use in assays) 851128-81-9P 851128-75-1P 851128-78-4P 851128-84-2P IT 851128-86-4P **851128-88-6P** 851128-94-4P (fluorinated resorufin compds. and their use in assays) ΙT 9003-99-0, Peroxidase (fluorogenic compd. reaction with peroxide in presence of; fluorinated resorufin compds. and their use in assays) 9003-99-0D, Peroxidase, conjugates with carrier IT 39391-18-9, Cyclooxygenase (fluorogenic compd. reaction with peroxide in presence of; fluorinated resorufin compds. and their use in assays) 7722-84-1, Hydrogen peroxide, analysis ΙT (fluorogenic compd. reaction with, in presence of peroxidase; fluorinated resorufin compds. and their use in assays) IT 14915-07-2, Peroxide (fluorogenic compd. reaction with, in presence of peroxidase; fluorinated resorufin compds. and their use in assays) IT 851128-96-6P (use in detg. cytotoxicity of test compds.; fluorinated resorufin compds. and their use in assays)

ANSWER 2 OF 4 HCA COPYRIGHT 2006 ACS on STN

141:93968 Hair dyeing compositions containing a

monoheteroyldiarylmethane direct dye or its leuco precursor. Guerin, Frederic; Lagrange, Alain (L'oreal, Fr.). Fr. Demande FR 2849373 Al 20040702, 74 pp. (French). CODEN: FRXXBL. APPLICATION: FR 2002-16851 20021230.

AB Hair dyeing compns. comprise a direct monoheteroyldiarylmethane dye and its leuco precursors. Thus, a formulation contained N-[4-[[4-(diethylamino)phenyl](4-oxo-4H-1-benzopyran-3-yl)methylene]-2,5-cyclohexadien-1-ylidene]-N-ethylethanaminium perchlorate 0.553, oleic diethanolamide 3, lauric acid 1, ethylene glycol monoethyl ether 5, hydroxyethyl cellulose 2, 2-amino-2-methyl-1-propanol 9.5, and water qs to 100 g. chloride 0.56, benzyl alc. 4.0, PEG 6.0, hydroxyethyl cellulose 0.7, alkyl polyglucoside 4.5, phosphate buffer 7, and water qs to 100 g.

IT 9003-99-0, Peroxidase 81769-84-8 81769-89-3 81769-90-6 81790-04-7

(hair dyeing compns. contg. monoheteroyldiarylmethane direct dye or its leuco precursor)

RN 9003-99-0 HCA

CN Peroxidase (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 81769-84-8 HCA

CN 1-Piperidinyloxy, 4-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl][3,5-bis(1,1-dimethylethyl)-4-oxo-2,5-cyclohexadien-1-ylidene]methyl]-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

RN 81769-89-3 HCA

CN 1H-Pyrrol-1-yloxy, 3-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl][3,5-bis(1,1-dimethylethyl)-4-oxo-2,5-cyclohexadien-1-ylidene]methyl]-2,5-dihydro-2,2,5,5-tetramethyl- (9CI) (CA INDEX NAME)

RN 81769-90-6 HCA

CN 1H-Pyrrol-1-yloxy, 3-[[3,5-bis(1,1-dimethylethyl)-4-oxo-2,5-cyclohexadien-1-ylidene][3,5-bis(1,1-dimethylethyl)-4-oxyphenyl]methyl]-2,5-dihydro-2,2,5,5-tetramethyl- (9CI) (CA INDEX NAME)

RN 81790-04-7 HCA

CN 1-Piperidinyloxy, 4-[[3,5-bis(1,1-dimethylethyl)-4-oxo-2,5-cyclohexadien-1-ylidene][3,5-bis(1,1-dimethylethyl)-4-oxyphenyl]methyl]-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

56413-29-7

56413-30-0

```
IC
     ICM
          A61K007-13
CC
     62-3 (Essential Oils and Cosmetics)
ΙT
     95-55-6D, o-Aminophenol, derivs.
                                          95-70-5, p-Toluenediamine
     106-50-3, p-Phenylenediamine, biological studies
                                                          106-50-3D,
     p-Phenylenediamine, derivs.
                                    108-45-2D, m-Phenylenediamine, derivs.
     108-46-3D, Resorcinol, derivs.
                                       123-30-8, p-Aminophenol
     123-30-8D, p-Aminophenol, derivs.
                                           124-43-6
                                                      591-27-5D,
                               2835-95-2, 5-Amino-2-methylphenol
     m-Aminophenol, derivs.
                                                       3810-38-6
     3486-48-4
                 3737-88-0
                              3737-89-1
                                           3737-91-5
                                           7722-84-1, Hydrogen peroxide,
     6411-50-3
                 6735-60-0
                              6837-66-7
     biological studies 9003-99-0, Peroxidase
     9035-73-8, Oxidase
                           9037-29-0, Oxygenase
                                                   10231-59-1
                                                                 13158-70-8
     13158-71-9
                  13158-72-0
                                13158-73-1
                                              15081-86-4
                                                            15082-04-9
                                                            18198-28-2
     17329-99-6
                  17330-00-6
                                17330-03-9
                                              17330-04-0
     18198-29-3
                  18198-30-6
                                18198-31-7
                                              22179-00-6
                                                            22179-01-7
     22196-95-8
                  23266-29-7
                                23266-30-0
                                              23266-31-1
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                  23266-34-4
                                23266-35-5
                                              23266-36-6
                                                            23297-28-1
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                                25361-34-6
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     23335-34-4
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     33609-83-5
                  34762-92-0
                                36525-76-5
                                              37111-44-7
                                                            38213-80-8
     38557-41-4
                  38557-42-5
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                                              38557-44-7
                                                            38557-45-8
     40683-08-7
                  40683-09-8
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                                                            40683-12-3
     40739-75-1
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                                42297-76-7
                                              42297-77-8
                                                            42297-78-9
                                              42297-82-5
                  42297-80-3
                                42297-81-4
                                                            42297-83-6
     42297-79-0
     42443-53-8
                  47334-92-9
                                47334-93-0
                                              47334-95-2
                                                            47433-65-8
                                                            47645-26-1
     47433-66-9
                  47569-88-0
                                47571-92-6
                                              47615-09-8
     47646-24-2
                  47699-20-7
                                47699-21-8
                                              47700-01-6
                                                            47701-02-0
     47725-05-3
                  47742-10-9
                                47742-82-5
                                              47789-57-1
                                                            47791-05-9
     47816-91-1
                  48230-04-2
                                48237-01-0
                                              49716-03-2
                                                           50548-08-8
     50584-48-0
                  50904-51-3
                                50904-52-4
                                              50904-53-5
                                                            50904-54-6
                                54111-86-3
                                              54117-49-6
                                                            54117-50-9
     51107-46-1
                  51107-47-2
     54117-51-0
                  54117-52-1
                                54117-53-2
                                              54117-54-3
                                                            55302-96-0,
                                                        56413-28-6
     5-N-(.beta.-Hydroxyethyl)amino-2-methyl phenol
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56413-31-1

56413-32-2

56413-33-3

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56413-37-7
                                                      56413-38-8
             56413-35-5
                           56413-36-6
56413-34-4
56413-39-9
             56523-96-7
                           56523-97-8
                                        56523-98-9
                                                      56524-08-4
                           56524-11-9
                                        57693-25-1
                                                      57693-26-2
56524-09-5
             56524-10-8
                                        61578-26-5
                                                      61937-91-5
57877-71-1
             61578-24-3
                           61578-25-4
61938-02-1
             61938-03-2
                           72828-90-1
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                                                      74567-64-9
                                        79377-98-3
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79377-85-8
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                           79377-92-7
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79395-69-0
81769-89-3 81769-90-6 81790-04-7
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                           83968-92-7
                                        84113-63-3
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83968-90-5
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94885-70-8
             94885-71-9
                           94885-72-0
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                                        94885-78-6
                                                      94885-79-7
94885-75-3
             94885-76-4
                           94885-77-5
96597-44-3
             96597-45-4
                           96597-49-8
                                        96622-84-3
                                                      97628-71-2
                                         104488-58-6
                                                        104488-59-7
97628-72-3
             97628-73-4
                           104038-58-6
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                             107278-34-2
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104511-49-1
              107278-33-1
                                           108403-62-9
                                                          108403-63-0
              107464-81-3
                             108403-61-8
107464-79-9
                                                          116915-58-3
                             108403-66-3
                                           112988-80-4
              108403-65-2
108403-64-1
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                                           118727-54-1
                                                          119482-85-8
117881-66-0
              117881-93-3
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                                           122235-20-5
                                                          124360-14-1
119570-73-9
              119570-76-2
                                                          181423-86-9
124360-15-2
              146091-29-4
                             156470-28-9
                                           181423-83-6
                                           181423-97-2
                                                          181424-03-3
181423-88-1
              181423-91-6
                             181423-94-9
181424-11-3
              181424-16-8
                             181424-17-9
                                           181424-22-6
                                                          181424-28-2
                                           181424-43-1
                                                          181424-48-6
              181424-34-0
                             181424-39-5
181424-29-3
181424-52-2
              181424-56-6
                             181424-60-2
```

(hair dyeing compns. contg. monoheteroyldiarylmethane direct dye or its leuco precursor)

140:289230 Fabric care compositions containing UV protectant, dye sequestrant, fabric softener etc. Adair, Matha J.; Finn, Leslie S.; Petrin, Michael J.; Rodriguez, Cheryl H.; Shanks, Philip C.; Van

ANSWER 3 OF 4 HCA COPYRIGHT 2006 ACS on STN

Petrin, Michael J.; Rodriguez, Cheryl H.; Shanks, Philip C.; Van Buskirk, Gregory; De Leo, Malcolm A.; Selbach, Hanneliese S.; Ochomogo, Maria G. (USA). U.S. Pat. Appl. Publ. US 2004063597 A1 20040401, 30 pp. (English). CODEN: USXXCO. APPLICATION: US

2002-259179 20020927.

AB A non-liq., liq., liq.-gel or gelled fabric care compn. comprises one or more fabric care enzymes effective for aiding in preventing pilling fuzzing, staining and other deterioration of fabric fibers during the wash process. The fabric care compn. also comprises one or more UV protectants for brightening and preventing light caused photo fading or other damage to fabrics. The fabric care compn. comprises one or more surface active dispersing, emulsifying and/or solubilizing agent principally comprised of surfactants, co-surfactants, hydrotropes and solvents selected to solubilize or stabilize the compn. The fabric care compn. also comprises one or more dye-transfer inhibitors, anti-redeposition agents or dye sequestrants to prevent re-deposition of dyes which have become transient from other fabrics. The fabric care compn. comprises one

or more dye, pigment and fabric color fixative or finish protectant to lock-in dyes and pigments to prevent their loss in quantity or quality during soaking or washing. The fabric care compn. optionally comprises one or more textile lubricant and/or textile softening agent to coat the textiles and reduce inter-fiber and fiber surface friction. The fabric care compn. also comprises one or more hardness and metal ion sequestrants and crystal growth inhibitors to bind free ions to prevent formation of insol. ppt. compds. The fabric care compn. also comprises one or more chlorine and/or active oxygen scavengers or neutralizers which act to neutralize oxidizing agents, i.e., those species with oxidn. The fabric care compn. optionally comprises one or more from the following: handling, storage, processing agents to modify elastic and viscous phase properties, anti-foaming or frothing agents, anti-microbial, anti-bacterial or anti-fungal agents, pH buffer, adjustment and/or modification, as needed, aesthetic dyes and/or fragrances.

IT **9005-25-8**, **Starch**, uses

(cationic, dye-transfer inhibitor; fabric care compns. contg. UV protectant, dye sequestrant, fabric softener etc)

RN 9005-25-8 HCA

CN Starch (8CI, 9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT 9003-99-0, Peroxidase

(dye-transfer inhibitor; fabric care compns. contg. UV protectant, dye sequestrant, fabric softener etc)

RN 9003-99-0 HCA

CN Peroxidase (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT 1643-20-5, Lauryl amine oxide

(nonionic surfactant; fabric care compns. contg. UV protectant, dye sequestrant, fabric softener etc)

RN 1643-20-5 HCA

CN 1-Dodecanamine, N, N-dimethyl-, N-oxide (9CI) (CA INDEX NAME)

IC ICM C12S009-00

INCL 510276000; 510392000

CC 46-5 (Surface Active Agents and Detergents)

IT Quaternary ammonium compounds, uses

((2-hydroxypropyl)methylditallow alkyl, chlorides, cationic fabric softener; fabric care compns. contg. UV

protectant, dye sequestrant, fabric softener etc) IT Oligosaccharides, uses (deriv., optionally alkoxylated, nonionic surfactant; fabric care compns. contg. UV protectant, dye sequestrant, fabric softener etc) Quaternary ammonium compounds, uses IT (dimethylditallow alkyl, chlorides, cationic fabric softener; fabric care compns. contg. UV protectant, dye sequestrant, fabric softener etc) 107-64-2, Distearyl dimethylammonium **chloride** 7212-69-3, IT Dioleyl dimethylammonium chloride 92888-37-4, Methyl bis(oleylamidoethyl)2-hydroxyethyl ammonium methyl sulfate 676162-67-7, Dimyristyl diethyl ammonium bromide (cationic fabric softener; fabric care compns. contg. UV protectant, dye sequestrant, fabric softener etc) 9005-25-8, Starch, uses IT (cationic, dye-transfer inhibitor; fabric care compns. contg. UV protectant, dye sequestrant, fabric softener etc) 9000-30-0, Guar gum 9002-89-5, Polyvinyl alcohol 9002-98-6 IT 9003-39-8D, Polyvinyl pyrrolidone, optionally deriv. 9004-32-4, Carboxymethyl 9003-99-0, Peroxidase cellulose 9004-42-6, Carboxyethyl cellulose 9004-67-5, Methyl cellulose 9005-32-7, Alginic acid 9045-81-2, Polyvinylpyridine-N-oxide 9035-73-8, Oxidase 12619-70-4, Cyclodextrins 25232-42-2, Polyvinyl imidazole 25608-40-6, Polyaspartic acid 26062-48-6, Polyhistidine 26063-13-8, Polyaspartic acid 26854-81-9, Polyhistidine 106392-12-5, Ethylene oxide-propylene oxide block copolymer 182482-80-0, Polyvinyl oxazolidone (dye-transfer inhibitor; fabric care compns. contg. UV protectant, dye sequestrant, fabric softener etc) 108-95-2D, Phenol, deriv., alkoxylated **1643-20-5**, Lauryl IT 13840-40-9, Phosphine oxide 26912-60-7 amine oxide (nonionic surfactant; fabric care compns. contg. UV protectant, dye sequestrant, fabric softener etc) 71-00-1, Histidine, uses 74-79-3, Arginine, uses 77-86-1, IT 111-42-2, Tris(hydroxymethyl)aminomethane 100-97-0, uses Diethanolamine, uses 141-43-5, Monoethanolamine, uses 9003-05-8 12125-02-9, Ammonium Sodium thiosulfate chloride, uses 24937-47-1, Polyarginine 25013-16-5, 25104-18-1, Polylysine Butylated hydroxyanisole 25212-18-4, Polyarginine 26336-38-9, Vinylamine homopolymer 38000-06-5, Polylysine (scavenger; fabric care compns. contg. UV protectant, dye

L49 ANSWER 4 OF 4 HCA COPYRIGHT 2006 ACS on STN 133:94512 Improved formulation for topical non-invasive application in

sequestrant, fabric softener etc)

vivo. Cevc, Gregor (Idea Innovative Dermale Applikationen G.m.b.H., PCT Int. Appl. WO 2000038653 A1 20000706, 73 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP8421 19981223. AB A formulation comprises mol. arrangements capable of penetrating pores in a barrier, owing to penetrant adaptability, despite the fact that the av. diam. of the pores is smaller than the av. penetrant diam., provided that the penetrants can transport agents or cause permeation through the pores after penetrants have entered The formulation comprises at least 1 consistency builder in an amt. that increases the formulation to maximally 5 Nm/s so that spreading over is enabled. The formulation also contains 1 antioxidant in an amt. that reduces the increase of oxidn. index to <100% per 6 mo and/or at least 1 microbicide in an amt. that reduces the bacterial count of 1 million germs added/g of total mass of the formulation to <100 in the case of aerobic bacteria, to <10 in the case of entero-bacteria, and to <1 in the case of Pseudomonas aeruginosa or Staphilococcus aureus, after a period of 4 days. Thus, a compn. contained soybean phosphatidylcholine 347, Tween-80 623, sodium dodecyl sulfate 30, benzyl alc. 50, clobetasol 17-propionate 25 and pH 6.5 50 mM phosphate buffer 9000 mg. IT 1643-20-5, Dodecyldimethylamine oxide 9004-34-6D, Cellulose, derivs., biological studies (penetrating formulation for topical non-invasive application in

1-Dodecanamine, N, N-dimethyl-, N-oxide (9CI) (CA INDEX NAME)

$$^{
m O}_{||}_{
m Me-N-(CH_2)_{11}-Me}$$

Me

RN

CN

vivo) 1643-20-5

HCA

RN 9004-34-6 HCA

CN Cellulose (8CI, 9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IC ICM A61K009-127

CC 63-6 (Pharmaceuticals)

Section cross-reference(s): 1

IT Quaternary ammonium compounds, biological studies

(alkylbenzyldimethyl, bromides; penetrating formulation for topical non-invasive application in vivo) Quaternary ammonium compounds, biological studies ΙT (alkylbenzyldimethyl, chlorides; penetrating formulation for topical non-invasive application in vivo) Quaternary ammonium compounds, biological studies IT (bromides; penetrating formulation for topical non-invasive application in vivo) IT Ouaternary ammonium compounds, biological studies (chlorides; penetrating formulation for topical non-invasive application in vivo) 50-06-6, Phenobarbital, biological studies 50-33-9, IT Phenylbutazone, biological studies 50-78-2, Acetylsalicylic acid 50-81-7, Ascorbic Acid, biological studies 50-99-7, Glucose, 52-67-5, Penicillamine 53-86-1, Indomethacin biological studies 54-64-8, Thiomersal 55-56-1, Chlorhexidine 54-05-7, Chloroquine 55-68-5, Phenylmercuric nitrate 56-81-5, Glycerol, biological studies 57-15-8, Chlorbutanol 59-02-9, .alpha.-Tocopherol 59-50-7, 4-Chloro-m-cresol 59-05-2, Methotrexate 60-00-4, EDTA, 61-68-7, Mefenamic acid 62 - 38 - 4, biological studies Phenylmercuric acetate 62-56-6, Thiourea, biological studies 64-17-5, Ethyl alcohol, biological studies 65-85-0, Benzoic acid, biological studies 67-63-0, Isopropyl alcohol, biological studies 67-68-5D, DMSO, alkyl derivs. 69-72-7, Salicylic Acid, biological 69-93-2, Uric acid, biological studies 70-18-8, Glutathione, biological studies 70-30-4, Hexachlorophene 81-24-3D, salts 81-25-4D, salts 83-44-3D, salts 83-89-6, 89-65-6 90-05-1, Guaiacol 86-74-8, Carbazole Quinacrine 90-34-6, Primaguine 94-13-3, Propylparaben 94-18-8, 94-26-8, Butylparaben 97-23-4, Dichlorophene Benzylparaben 99-50-3, Protocatechuic Acid 99-76-3, Methylparaben 100-51-6, Benzyl alcohol, biological studies 102-98-7, Phenylmercuric borate 103-90-2, Acetaminophen 107-15-3D, Ethylenediamine, derivs. 107-21-1, Ethylene glycol, biological studies 110-27-0, Isopropyl myristate 110-44-1, Sorbic acid 112-53-8, 1-Dodecanol 112-80-1, Oleic acid, biological studies 118-42-3, Hydroxychloroquine 119-13-1, .delta.-Tocopherol 120-47-8, 121-79-9, Propyl Gallate Ethylparaben 121-33-5, Vanillin 122-39-4, Diphenylamine, biological studies 123-03-5, Cetylpyridinium chloride 123-31-9, Hydroquinone, biological studies 128-37-0, BHT, biological studies 129-20-4, 137-66-6 138-14-7, Desferal 141-78-6, EtOAc, Oxyphenbutazone 143-19-1, Sodium oleate 143-28-2, Oleyl biological studies 148-03-8, .beta.-Tocopherol 149-91-7, Gallic Acid, alcohol biological studies 151-41-7, Lauryl sulfate 302-95-4, Sodium deoxycholate 327-97-9, Chlorogenic acid 331-39-5, Caffeic acid 360-65-6D, salts 446-86-6, Azathioprine 475-31-0D, salts

476-66-4, Ellagic Acid 484-78-6, 3-Hydroxykynurenine 490-79-9,

Gentisic acid 500-38-9, Nordihydroguaiaretic Acid 516-50-7D, 525-66-6, Propranolol 530-57-4, Syringic Acid 530-59-6, salts 530-78-9, Flufenamic acid 534-61-2, IsoChlorogenic Sinapic acid 538-71-6, Phenododecinium bromide 548-93-6, 3-Hydroxyanthranilic acid 616-91-1, N-Acetylcysteine 621-82-9, Cinnamic acid, biological studies 629-25-4, Sodium laurate 822-17-3, Sodium linoleate 635-65-4, Bilirubin, biological studies 1118-68-9D, Dimethylglycine, alkyl derivs. 1135-24-6, Ferulic acid 1319-77-3, Cresol 1643-20-5, Dodecyldimethylamine oxide 1948-33-0, tert-Butylhydroquinone 1951-25-3, Amiodarone 3650-09-7, Carnosic acid 2002-22-4D, derivs. 2495-84-3 5677-55-4, Ubiquinol-10 4353-06-4 5432-30-4 5957-80-2, 7235-40-7, .beta.-Carotene 7347-25-3, Sodium taurate Carnosol 7616-22-0, .gamma.-Tocopherol 7631-90-5, Sodium bisulphite 7681-57-4, Sodium metabisulfite 7747-53-7 9000-07-1, Carrageenan 9000-30-0, Guar-qum 9000-65-1, Tragacanth 9000-69-5, Pectin 9001-05-2, Catalase 9002-88-4, Polyethylene 9002-89-5, Polyvinyl alcohol 9002-92-0, Polyethylene glycol dodecyl ether 9002-96-4 9003-39-8, Polyvinylpyrrolidone 9004-32-4, Carboxymethyl cellulose sodium salt 9004-34-6D, Cellulose, derivs., biological studies 9004-61-9, Hyaluronic Acid 9004-62-0, Hydroxyethyl cellulose 9004-64-2, Hydroxypropyl **cellulose** 9004-65-3, Hydroxypropylmethyl cellulose 9004-67-5, Methyl 9004-98-2, Polyethylene glycol oleyl ether cellulose 9004-99-3, Myrj 45 9005-32-7, Alginic acid 9005-64-5, Tween 20 9012-36-6, Agarose 9012-76-4, Chitosan 9005-65-6, Tween 80 9036-19-5, 9013-66-5, Glutathione peroxidase Polyethylene glycol octylphenyl ether 9043-30-5, Polyethylene glycol isotridecyl ether 9054-89-1, Superoxide dismutase 9086-85-5, Poly(hydroxypropyl) methacrylate 10540-29-1, Tamoxifen 12041-76-8, Dichlorobenzylalcohol 11138-66-2, Xanthan 15687-27-1, Ibuprofen 15307-86-5, Diclofenac 16409-34-0, Sodium glycodeoxycholate 16690-40-7 18175-45-6, Sodium elaidate 18472-51-0, Chlorhexidine gluconate 18683-91-5, Ambroxol 19767-45-4, Mesna 20283-92-5, Rosmarinic acid 20902-45-8, Penicillamine disulfide 21829-25-4, Nifedipine 22071-15-4, 22204-53-1, Naproxen 22494-42-4, Diflunisal Ketoprofen 23288-49-5, Probucol 25013-16-5, BHA 25014-41-9, 25429-38-3, 25249-16-5 25322-68-3, PEG Polyacrylonitrile 26570-48-9, Coumaric acid 25655-41-8, Povidone-iodine Polyethylene glycol-diacrylate 26746-38-3, Di-tert-butylphenol 27306-76-9, Polyethylene glycol cetyl stearyl ether Polyethylene glycol myristyl ether 29122-68-7, Atenolol 29349-22-2, Chlorobenzyl alcohol 33425-76-2 36322-90-4, 36413-60-2, Quinic Acid 37640-71-4, Aprindine Piroxicam 53188-07-1, Trolox 53584-19-3 55985-32-5, Nicardipine 63675-72-9, Nisoldipine 66085-59-4, Nimodipine 59227-89-3, Azone

68047-06-3, Hydroxytamoxifen 68555-46-4 75530-68-6, Nilvadipine 77400-65-8, Asocainol 85261-20-7, Decanoyl N-methylglucamide 87246-72-8 88306-53-0 90522-12-6 91729-95-2, Rosmaridiphenol 99716-88-8, Methallylsulfonic acid homopolymer 106392-12-5, Poloxamer 110101-67-2, U74006F 118457-14-0, Nebivolol 121869-32-7 148081-72-5, 1-O-Hexyl-2, 3, 5-trimethylhydroquinone (penetrating formulation for topical non-invasive application in vivo)